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MULTI-DIMENSIONAL TUNNELLING AND COMPLEX MOMENTUM

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ABSTRACT

We examine the problem of modelling tunnelling phenomena in more than one dimension. We find that existing techniques are inadequate in a wide class of situations, due to their inability to deal with concurrent classical motion. We show how to generalise these methods to allow for complex momenta, and demonstrate the improved techniques with a selection of illustrative examples. We comment on possible applications.

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Tunnelling is perhaps one of the more versatile concepts of quantum theory. It may be used in tunnelling microscopy¹, or in describing a phase transition in the universe²! But, whatever tunnelling problem one wishes to address, all have in common the idea that two regions of space classically separated by a potential barrier are not quantum mechanically isolated, provided the barrier separating the two is finite. The reason is that in the classically forbidden régime the probability density is non-zero, although exponentially damped.

Such is the simple picture. In practice however, calculating a tunnelling amplitude accurately is not so easy, except in a range of special cases, essentially one-dimensional problems or problems which can be recast as such. Recently, in considering inflationary scenarios, people have been examining models containing not only an inflaton scalar field responsible for the false vacuum energy, but also an additional scalar field, either by extending the gravitational sector, as in extended³ or hyperextended⁴ inflation, or by including an extra scalar field, as in double field inflation⁵. These ideas have in common the notion of a single field whose tunnelling is influenced by the classical evolution of a second field. This allows for a time dependent nucleation rate which resolves several problems with the old inflationary models. To date, most calculations⁴⁻⁷ have involved a “freezing out” of the second field, merely using it to provide dynamical evolution parameters in the one-dimensional problem. Since most tunnelling calculations involve stationary state Euclidean time techniques, these more complex multi-dimensional models beg the question as to whether such techniques are really valid when there is classical evolution. The aim of this paper is to approach this problem in a way that treats both types of evolution on an equal footing.

In this paper, we explore this question for the test case of quantum mechanical tunnelling, and consider a variety of illustrative potentials. We concentrate on the stationary phase or quasi-classical approximation, examining how, and under precisely what conditions this may be applied. In particular, we try to avoid assigning Euclidean time any preferred status, keeping it firmly in the category of an optional mathematical tool. In dealing with this more general class of problems, we find that we have to modify the WKB matching conditions to allow for the passage of real momentum under a barrier and complex momentum beyond. This naturally increases the complexity of the process of solving for the wave function under the barrier and beyond. We develop a method for solving these two problems and apply it to a variety of two-dimensional examples.

The layout of the paper is as follows. We begin by reviewing the quasi-classical approximation, and what limitations it places on the type of tunnelling wave functions to be considered. We also review the role of Euclidean time, and highlight the problems of

trying to apply these techniques to more general multi-dimensional barriers. This leads us to our description of the identification of turning points in WKB solutions and derivation of appropriate matching conditions. We then solve the Schrödinger equation under the barrier in the stationary phase approximation. Finally, we apply our techniques to a few simple, but illustrative, examples.

1. Tunnelling and the Quasi-Classical Approximation.

Before reviewing the quasi-classical approximation, we will recap on what is usually meant by “tunnelling”. Tunnelling amplitudes for scattering problems are reasonably well defined as the ratio of the amplitudes of the emergent and incident wave functions. For ‘stationary’ problems (a particle ‘tunnelling’ from one well or channel to another) we will consider a particle to be tunnelling out of its initial well if the probability of finding it in that well or channel goes predominantly as $e^{-\Gamma t/\hbar}$. Γ is the tunnelling amplitude.

Now let us review the quasi-classical approximation⁸. As the name suggests, this approximation extracts the leading order “classical” behaviour of the system, and is only valid when the de-Broglie wavelengths of the particles are small compared to the characteristic scales of the motion. Explicitly, if we set

$$\psi = e^{i\sigma/\hbar} e^{-iEt/\hbar} \quad (1.1)$$

the Schrödinger equation gives

$$\frac{1}{2m}(\nabla\sigma)^2 - \frac{i\hbar}{2m}\nabla^2\sigma = E - U(\mathbf{x}) \quad (1.2)$$

as the equation of motion for σ . The quasi-classical approximation is that we drop the $O(\hbar)$ term in (1.2), which clearly requires that $|\nabla\sigma|^2 \gg \hbar|\nabla^2\sigma|$. If we identify the momentum \mathbf{p} with $\nabla\sigma$, we see automatically that the approximation is invalid for very small momenta, i.e. in regions where $E \sim U$. Thus a classical particle at rest has no stationary quasi-classical counterpart. However, what is perhaps less obvious is that this approximation also breaks down for more general turning points, when the momentum becomes parallel to the potential. We will discuss this point in more detail later.

In general, if we are given σ_i at some initial point \mathbf{x}_i , we may write the solution for σ as

$$\sigma(\mathbf{x}) = \int_{\mathbf{x}_i}^{\mathbf{x}} \nabla\sigma \cdot d\mathbf{l} + \sigma_i \quad (1.3)$$

where $d\mathbf{l}$ is any path interpolating between \mathbf{x}_i and \mathbf{x} . This is all very well, but what is $\nabla\sigma$? The Schrödinger equation is a scalar equation, relating the magnitude of $\nabla\sigma$ to U , yet we

presumably need to solve it throughout some multi-dimensional region of space. Banks, Bender and Wu⁹ solved this problem for the case of tunnelling from a localised state in more than one dimension. We will summarise their approach (and others¹⁰) here, before going on to discuss tunnelling from non-localised states.

Essentially, they treated (1.2) rather like a geodesic problem, setting $\nabla\sigma \propto d\mathbf{l}$, thus making (1.3) a scalar integral with respect to the length parameter along the path. This requires that $\nabla\sigma$ has constant phase, and hence is purely real or imaginary, the latter case corresponding to tunnelling. To solve this tunnelling problem, they set $\sigma = ig$ and thus obtain to lowest order in \hbar

$$(\nabla g)^2 = 2m(U - E) \quad (1.4a)$$

$$\Rightarrow \quad \sigma = i \int^{\mathbf{x}_f} \sqrt{2m(U - E)} d\mathbf{l}, \quad (1.4b)$$

where \mathbf{l} is the path which minimises the integral, the *escape path*, and \mathbf{x}_f is the point of emergence of that path into the classical régime. In this case, it is clear how to solve (1.4a) exactly, however a common alternate method, indispensable in field theory, uses a Euclidean time description.

First we replace $\mathbf{p}_e = \nabla g$ in (1.4a), which yields

$$\mathcal{H} = -\frac{1}{2m} \mathbf{p}_e^2 + U = E. \quad (1.5)$$

This can then be interpreted as a Hamiltonian problem of particle motion in the (inverted) potential $-U$. We then see that there is a non-trivial solution, $\mathbf{x}(\tau)$, which interpolates between the initial position of the particle and its position of emergence from the barrier. With our Hamiltonian interpretation we identify $\dot{\mathbf{x}}(\tau)$ with \mathbf{p}_e , and τ is thought of as a time parameter. The identification of τ as a Euclidean time comes from noting that $\frac{dz}{dt} = \mathbf{p} = i\mathbf{p}_e = i\dot{\mathbf{x}}(\tau)$, thus $\tau = it$. Solving the Hamiltonian problem along the trajectory gives:

$$-\frac{1}{2} \dot{\mathbf{x}}(\tau)^2 + U = E \quad (1.6)$$

hence

$$\sigma = -i \int \mathbf{p} \cdot d\mathbf{l} = -i \int \mathbf{p} \cdot \dot{\mathbf{x}} d\tau = i \int 2(U - E) d\tau. \quad (1.7)$$

The advantage of this approach is that it provides a straightforward means of calculating the escape path and action in terms of a classical mechanics problem, the disadvantage is that it introduces a fictitious time parameter along that path which can introduce conceptual confusion in trying to interpret what the 'particle' is 'doing'. For example, a

statement often made is that because Euclidean time is somehow orthogonal to real time, tunnelling happens instantaneously; this is rather confusing. Tunnelling is a statement on the dynamical evolution of the wave function according to quantum mechanics, whereas to say “happens instantaneously” suggests an observation, i.e. an interaction with the system. The only process one can label as tunnelling is the quantum mechanical leakage of probability across a barrier which is distinct from the path of a classical particle, and also distinct from an observation of the particle on the other side. The actual question of tunnelling time is an extremely subtle and complicated one (for a review see Hauge and Stovneng¹¹), and to some extent depends on how one chooses to formulate it. However, what one can say is that a probability density at time $t_0 + \epsilon$ at some point in space other than that at which a particle was observed at time t_0 is not a demonstration of instantaneous motion, but rather a reflection of the dynamics of the Schrödinger equation.

Before going on to describe a more general approach to ‘escape paths’ we will make the obvious remark (which Goncharev and Linde¹² discuss in more detail) that the standard Banks-Bender-Wu method requires that $(\nabla g)^2 = \dot{\mathbf{x}}^2 \rightarrow 0$ at each end of the escape path, otherwise the solution cannot be matched with a classical ‘real time’ solution in the asymptotic regime. In the case of escape from a localised state, this can be guaranteed, since one end of the escape path is necessarily fixed and the other end is varied freely to find the minimum action, therefore we are free to set $\dot{\mathbf{x}}^2 = 0$ at each end. However, in a more general scenario, such as channel-channel tunnelling, this need not be the case. Both ends of the escape path can now be moved, and hence it requires *two* initial conditions (rather than one as in the previous case) to fix the start of the path. Thus, since our equations of motion are second order, we have used up our quota of boundary conditions, and we just have to hope that in varying our other endpoint we ‘hit lucky’. Unfortunately, from (1.6) we see that $\dot{\mathbf{x}} = \nabla U$ along the path, thus if U is for example monotonically increasing parallel to the barrier, $\dot{\mathbf{x}}$ has a strictly positive component in that direction. Therefore $\dot{\mathbf{x}}^2$ can never be zero at both ends of any trajectory and the Banks-Bender-Wu method is not applicable.

Another disadvantage of this approach is that it makes no allowance for the transport of real momentum under a barrier. In the case of a continuous symmetry it is clear that such transport does occur, since the extra degrees of freedom decouple from the problem, and the wave function is merely a product of a tunnelling wave function with suitable transverse momenta eigenfunctions. However, trying to incorporate this into a fully Euclidean picture is not so easy¹³. And of course we have totally ignored the problem of picking an initial position from which to integrate, since we can only localise a particle at the expense of information about its momentum. We clearly need a more general picture of tunnelling.

As we have noted above, in the approach of Banks, Bender and Wu, we must take space to be divided into regions in which $\nabla\sigma$ is entirely real or entirely imaginary; this is what allows us to make the identification of $\nabla\sigma$ with some \dot{x} ("time"). Clearly we then need \dot{x} to vanish on the boundaries where $\nabla\sigma$ changes from real to imaginary, but this obviously means that we have restricted ourselves to a certain subset of problems. As we have seen, it is not difficult to find a potential which does not fit into this subset. We must find an approach which allows for complex momentum as well as dealing with the problem of matching between classical and tunnelling régimes. This is what we will now develop.

2. Tunnelling with classical motion - general formalism.

We now turn to how we can modify the escape path techniques for more general potentials. The class of potentials we will be interested in are ones which contain two channels (or asymptotic regions) separated by some barrier in the 'x'-direction. We envisage that this barrier has some arbitrary y -dependence, but that this is secondary to the height of the barrier. Our main assumption, other than that of quasi-classicality, is that this barrier is always sufficiently high so that the division between 'classical' and 'tunnelling' motion is clear, i.e. $U \gg E$.

Recall that the essential problem of tunnelling with classical motion is twofold. First the transition from classically allowed to classically forbidden regimes is no longer characterised by real momentum becoming imaginary (or $E \sim U$): the momentum retains both real and imaginary pieces. Secondly, because the 'momentum' is now complex, the evolution equations become more complicated. The first point, deciding on matching conditions, is crucial; we may fix $(\nabla g)^2 = 0$ as we enter the barrier, but we must be able to interpret emergent solutions with non-zero ∇g .

In order to deal with complex momentum in the quasi-classical approximation, we rewrite (1.2) in terms of the real variables f and g , where $\sigma = f + ig$:

$$(\nabla f)^2 - (\nabla g)^2 + \hbar \nabla^2 g = 2m(E - U) \quad (2.1a)$$

$$2\nabla f \cdot \nabla g - \hbar \nabla^2 f = 0, \quad (2.1b)$$

this latter equation representing the constraint that the probability current, $\mathbf{j} = e^{-2g/\hbar} \nabla f$, is divergence free.

We now turn to the problem of matching conditions: where they should be applied, and how to determine them. First let us describe how to identify a turning point. Physically, the breakdown of the quasi-classical condition occurs when the de-Broglie wavelength of a particle becomes comparable to the physical scales of the potential. In problems where the momentum changes from being totally real to totally imaginary (or vice versa), this

is characterised by $E \sim U$. However, if we wish to allow simultaneous 'classical' evolution with tunnelling (i.e. complex momenta) then we must be more specific about the quantum to classical transition.

In the 'classical' régime we expect the variation of the phase of the wave function to dominate, whereas in the tunnelling régime the variation of the amplitude should be dominant. In each of these régimes, the quasi-classical condition breaks down when

$$|\nabla\sigma|^2 \sim \hbar|\nabla^2\sigma| \quad (2.2a)$$

in other words when

$$\begin{aligned} (\nabla f)^2 &\sim \hbar\nabla^2 f \\ (\nabla g)^2 &\sim \hbar\nabla^2 g. \end{aligned} \quad (2.2b)$$

These relations are satisfied either when $|\nabla f|$ or $|\nabla g|$ are small, i.e. when $E \sim U$, or when $|\nabla^2 f|$ or $|\nabla^2 g|$ become large, this latter situation occurring near generic turning points of the motion, approximately when the momentum becomes essentially orthogonal to the gradient of the potential. To see why this is, let us consider an incoming plane wave scattering off some barrier. The integral curves of ∇f trace out the path that a classical particle would follow in that potential. The breakdown of the approximation occurs when neighbouring, initially parallel, trajectories cross. (These can be either f -lines or g -lines.) The set of points where rays cross each other is referred to as a caustic and it is at these points that the approximation breaks down due to $\nabla^2 f$ (or $\nabla^2 g$) becoming unbounded. (In the path integral language, as we pass through the caustic the path changes from a minimum of the action, S , to a saddle point; that is one of the eigenvalues of $\delta^2 S$ becomes negative. In the expression for the propagator there is a term of the form $(\det \delta^2 S)^{-\frac{1}{2}}$ which diverges¹⁴.) The matching conditions should strictly be applied along the caustics of the f or g curves. However, since the barrier is assumed to be slowly varying along its length compared with its steepness, this actually coincides with the turning point of the f -line, when the momentum is orthogonal to ∇U .

The matching conditions in the situation $E \sim U$ are the standard matching conditions, that is, our initial conditions for integrating away from the turning point \mathbf{x}_0 are $g = 0$, $\nabla g = 0$, $\nabla f = 0$ if matching from classical to tunnelling, and $g = g(\mathbf{x}_f)$, $\nabla g = 0$, $\nabla f = 0$, if matching from tunnelling to classical at \mathbf{x}_f . In the second case, where there is some transverse momentum, then continuity of the wave function demands that the momentum parallel to the barrier is preserved. If this momentum is entirely real (or imaginary) the orthogonal part is matched as before. More precisely, the wave-function is given locally by

$$\psi = e^{\frac{i\hbar x}{k}} \text{Ai}(\hbar^{-\frac{2}{3}}(2mU_x)^{\frac{1}{3}}x), \quad (2.3)$$

where $\text{Ai}(x)$ is the Airy function. This gives an extra phase of $e^{\frac{i\pi}{2}}$ between the incident and reflected wave, which is a generic feature at such turning points and can be traced back to the change of phase in the determinant factor of the propagator caused by reversing one of the eigenvalues of $\delta^2 S$.

In the case where the incident wave has complex parallel momentum, $a_y + ib_y$, we might expect that

$$\psi = e^{\frac{i}{\hbar}(a_y + ib_y)y} \text{Ai} \left(\hbar^{-2/3} (2mU_x)^{1/3} \left(x + \frac{E - \frac{1}{2m}(a_y + ib_y)^2}{U_x} \right) \right). \quad (2.4)$$

However, using the asymptotic expansion for the Airy function, we find that the momentum of ψ in the x -direction is given by the energy equation

$$p_x^2 + (a_y + ib_y)^2 = 2m(E - U(x)), \quad (2.5)$$

hence if $a_y, b_y \neq 0$ p_x can never vanish. Returning to the functions f and g in equation (2.1a), we see that whenever the distance between the f -curves scales as d along their length, ∇g scales as d^{-1} , thus as we approach a ‘caustic’ of f -lines, $d \rightarrow 0$ and ∇g diverges, *unless* it happens to be zero. We can therefore think of the $(\nabla g)^2$ term as a repulsive potential between the f -lines, which provides a smooth transition between different régimes of our approximation.

In the examples that we consider the walls of the barrier are step-functions. In this simplified situation, we fix the (possibly complex) parallel momentum, and then compute the momentum perpendicular to the barrier using equations (2.1a,b), choosing the solution corresponding to an exponentially decaying wave-function under the barrier and an outgoing wave at the far side. In both cases, if we label the incoming and outgoing perpendicular component of the (complex) momentum by k_I and k_0 respectively, then a trivial calculation matching the wave-function and its derivative at the boundary shows that the reflected and transmitted waves have coefficients relative to the incident wave of

$$\frac{k_I - k_0}{k_I + k_0}, \frac{2k_I}{k_I + k_0} \quad (2.6)$$

respectively. Normally, the wave reflected from the incident decaying wave under the barrier is only an exponentially small correction (associated with multi-instanton solutions) to the wave-function, and so is generally disregarded in what follows, although it is responsible for the very small but non-zero ‘tunnelling component’ of the probability current.

Now that we have initial conditions for ∇g and ∇f under the barrier, and also at the far edge of the barrier, let us turn to the equations of motion.

Since we are assuming $E \ll U$, ∇g is clearly dominant under the barrier, however, this does not mean that we can neglect ∇f as an $O(\hbar)$ correction, otherwise we would use existing techniques. Instead we want to consider a situation where $\hbar \ll \frac{E}{U} \ll 1$, therefore we adopt a step by step procedure in solving

$$(\nabla g)^2 = 2mU - (2mE - (\nabla f)^2) \quad (2.7a)$$

$$\nabla f \cdot \nabla g = 0, \quad (2.7b)$$

bearing in mind that $(\nabla f)^2$, E are of the same order, and small compared with $(\nabla g)^2$, U .

The first step is to find the leading behaviour, that is, to solve

$$(\nabla g)^2 = 2mU. \quad (2.8)$$

This is solved using the existing techniques: we use the momentum transfer equation

$$\nabla \nabla_g \nabla g = m \nabla U \quad (2.9)$$

to find the integral curves of ∇g , and then integrate the scalar g along them:

$$g = \int_{x_0}^x \sqrt{2mU} \, ds \quad (2.10)$$

This gives us the solution to leading order. The next step is to use the initial conditions for ∇f to integrate (2.7b) through the barrier, since (2.7b) merely tells us that f is constant along g -lines: $f = f(\varphi)$ where $y_0 = \varphi(x, y)$ are the integral curves of g . Finally, we input this solution for f back in to (2.7a) to obtain the correct form of g to order E .

Now that we have a systematic method for solving underneath the barrier, an apparently reasonable question to ask would be what the actual flows of the particles were across the barrier. This, as it turns out, is a very difficult question to address, since it tries to relate a classical notion (a path) to a classically forbidden régime. Even setting aside such interpretive reservations, we see that our solution *as it stands* cannot represent tunnelling, since the probability current, $\mathbf{j} = e^{2g/\hbar} \nabla f$, is orthogonal to the integral curves of g and can therefore never leave the turning point. Clearly our solution is incomplete, since we know that particles do in fact tunnel, albeit with a very small amplitude. Let us first highlight a 'trick' by which we may obtain the form of the probability current before discussing its true origin and therefore limited interpretational value.

Consider first (2.1b) in one dimension. If we were to expand f in powers of \hbar we would conclude that $f = 0$. However if we directly solve (2.1b), we obtain

$$f'_T = f'_T(x_f) e^{2(g-g_f)/\hbar}. \quad (2.11)$$

Thus, we find that as well as the zero solution, we also have a non-zero g -dependent phase under the barrier. This suggests that in general the probability current along a g -line is

$$j_T \propto K e^{-2g(x_f)/\hbar} \quad (2.12)$$

a constant. We also have an order of magnitude estimate of the phase change along a g -line as $\hbar K$, where K is the outgoing momentum. Note that all the phase change takes place at the boundaries of the barrier, therefore to get the exact phase change we should look at the matching conditions. In the case of a step function, (2.6) implies

$$\Delta f_T = \Theta = \arg \left\{ \frac{2k_I}{k_O + k_I} \bigg|_N \frac{2k_I}{k_O + k_I} \bigg|_F \right\} \quad (2.13)$$

where the subscripts N and F refer to the near and far sides of the barrier respectively. An obvious point which we will nonetheless make is that if a path does not emerge from under a barrier, g increases without limit along that path, therefore the appropriate solution for f_T is the zero solution. This implies that no tunnelling can occur along such a path.

It would be nice to associate this probability current with the path of the particles, however, this would be hopelessly incorrect. We can only associate the probability current with a path if we have a single WKB-like wave function. Once we have a superposition of wave functions, such as incoming and outgoing waves, the probability current only represents a nett flow due to the interference between the various waves. In the case of real momenta, we can directly sum the probability current associated with each wave function to get the nett current. With complex momenta however, which unfortunately is precisely what we are interested in, it is the interference which gives the probability current. Thus, although this trick which we have illustrated does extract a probability current from a complex momentum wave function, the non-vanishing of this current relies crucially on the existence of a point of emergence for this wave function into the classical régime, and this is exactly equivalent to the existence of another, exponentially growing, branch of the solution. As such ∇f_T cannot be interpreted as a flow of particles under the barrier, but rather as a shorthand way of estimating the multi-instanton corrections which does in fact give the correct order of magnitude for the tunnelling current (although it is out by a factor of order unity).

Finally, before investigating a few concrete examples, we should summarise the limits to our approximation. First, we have assumed $E \ll U$ in order to facilitate the solution of (2.1) as an expansion in E/U . Our second main assumption involves the matching conditions in terms of the local orthogonal coordinates along the caustic, this requires that

the caustic not be too strongly curved which translates into a restriction on $U_{,yy}$. From (2.4) we see that the quasi-classical approximation is invalid for $|x| \leq \hbar^{2/3}(2mU_{,x})^{-1/3}$. This gives a rough order of magnitude limit $U_{,yy} \leq \hbar^{-4/3}(2mU_{,x})^{2/3}$, which one can substantiate with a more careful calculation. This shows that our turning point treatment is generically valid. In practise, calculational complexity will be the limiting factor for $U_{,yy}$ - curved caustics are more difficult to deal with.

3. Plane wave scattering - examples.

In order to examine the flows of the wave function we first consider a steady state flux of particles impinging on a variety of barriers, that is, $\psi_{\text{in}} = e^{ik \cdot x/\hbar}$. We do this because we no longer have localised quasi-classical states in the direction of classical motion. We follow the wave function under the barrier and out into the second 'classical' regime. After calculating the form of the tunnelled wave function, we use the momentum eigenstates to build the physically more realistic situation of a Gaussian wave packet hitting the barrier. This more realistic scenario allows us to highlight the existing controversy of tunnelling times for the square barrier, as well as illustrating some interesting new properties of more general barriers.

To illustrate our techniques we have chosen three examples in order of increasing complexity. We begin with the simplest possible two-dimensional potential - a separable square barrier. This allows us to check our calculations against an exact solution, and also leads naturally to the second example: a square barrier of varying width. Finally, we consider a square barrier of fixed width and varying height. These latter two potentials demonstrate some very peculiar scattering properties as we shall see.

Example 1: $U(x) = V\Theta(x)\Theta(a-x)$.

For this potential we know the exact form of the stationary eigenfunctions:

$$\psi(x) = e^{ip_2 y/\hbar} \psi_{p_1}(x) \quad (3.1)$$

where

$$\psi_{p_1}(x) = \begin{cases} e^{ip_1 x/\hbar} - \frac{1}{2}iT\left(\frac{\kappa}{p_1} + \frac{p_1}{\kappa}\right)e^{ip_1 a/\hbar}e^{-ip_1 x/\hbar} \sinh \kappa a/\hbar & x < 0 \\ \frac{1}{2}Te^{ip_1 a/\hbar} \left[\left(1 + \frac{ip_1}{\kappa}\right)e^{-\kappa(a-x)/\hbar} + \left(1 - \frac{ip_1}{\kappa}\right)e^{\kappa(a-x)/\hbar} \right] & 0 \leq x \leq a \\ Te^{ip_1 x/\hbar} & x > a. \end{cases} \quad (3.2)$$

is the usual one-dimensional square barrier wave function, with

$$p_1^2 = 2mE - p_2^2 \quad \kappa^2 = 2mV - p_1^2$$

$$T = e^{-ip_1 a/\hbar} \left(\cosh \kappa a/\hbar - \frac{i}{2} \left(\frac{p_1}{\kappa} - \frac{\kappa}{p_1} \right) \sinh \kappa a/\hbar \right)^{-1} \quad (3.3)$$

It will be convenient to rewrite this transmission coefficient as

$$T = \frac{2p_1\kappa}{D} e^{-ip_1 a/\hbar} e^{-i\Theta/\hbar} \quad (3.4)$$

where

$$D^2 = 4p_1^2 \kappa^2 + 4m^2 V^2 \sinh^2 \kappa a/\hbar \quad (3.5)$$

gives some measure of the transition amplitude, and

$$\frac{\Theta}{\hbar} = \tan^{-1} \left\{ \frac{\kappa^2 - p_1^2}{2p_1\kappa} \tanh \frac{\kappa a}{\hbar} \right\} \quad (3.6)$$

gives the 'transition phase'. This latter quantity is important in discussing some interpretations of the tunnelling time.

For $V \gg E$ we see that

$$D \sim 2mV \sinh \frac{\kappa a}{\hbar} \simeq mV e^{\kappa a/\hbar} \quad (3.7a)$$

$$\frac{\Theta}{\hbar} \sim \tan^{-1} \frac{\kappa}{2p_1} \simeq \frac{\pi}{2} - \frac{2p_1}{\kappa} \quad (3.7b)$$

and hence

$$T \sim \frac{2p_1\kappa}{mV} e^{-\kappa a/\hbar} \exp \left\{ \frac{-ip_1 a}{\hbar} - \frac{i\pi}{2} + \frac{2ip_1}{\kappa} \right\} \quad (3.8)$$

Comparing the transmitted solution with the incident solution, we see that the transmission amplitude, $|T|$, is given approximately by $\frac{4p_1}{\kappa} e^{-\kappa a}$ (having set $\kappa \sim \sqrt{2mV}$) and that the transmitted wave acquires a phase $(\frac{-p_1 a}{\hbar} - \frac{\pi}{2} + \frac{2p_1}{\kappa})$.

To solve the Schrödinger equation using a quasi-classical approach is in this case very straightforward since U is a function of one variable only. The solution of (2.7a) to leading order is $g = \sqrt{2mV}x$. Equation (2.7b) then implies that $f = p_2 y$. Equation (2.7a) then implies that $g = \sqrt{2m(V - E) + p_2^2} x = \kappa x$ as required.

To solve in the asymptotic régime we note that since $\nabla g = 0$ along $x = a$, g must be a constant, g_f , and therefore ∇f returns to its original value (p_1, p_2) . To find the phase shift across the barrier, Θ , we use (2.13) and obtain $\Delta f_T = \Theta = \tan^{-1} \frac{-\kappa}{2p_1}$, in agreement with (3.7b). Thus, integrating out from $x = a$, we obtain

$$g = \kappa a \quad (3.9a)$$

$$f = p_2 y + p_1(x - a) + \hbar\Theta \quad (3.9b)$$

in agreement with the exact solution.

Now we will attempt to solve for potentials which have a small y -dependence included:

Example 2: $U_2(x) = V\Theta(x)\Theta(a - x - \epsilon y)$.

This represents a barrier of constant height and varying thickness. Clearly, since our initial conditions for integrating under the barrier are the same as for the first example, the solution for f and g under the barrier is the same:

$$f = p_2 y, \quad g = \sqrt{2m(U - E) + p_1^2} x = \kappa x \quad (3.10)$$

To find the solution in the asymptotic region, we must recall the boundary conditions to be applied at the far edge of the barrier: $\nabla f_{||}$, $\nabla g_{||}$ are preserved. Now, if we assume that $\epsilon \ll 1$, and only keep terms of order ϵ , then the tangent and normal vectors to the far surface are, respectively,

$$\mathbf{T} = \begin{pmatrix} -\epsilon \\ 1 \end{pmatrix} \quad \mathbf{N} = \begin{pmatrix} 1 \\ \epsilon \end{pmatrix}. \quad (3.11)$$

Therefore

$$\nabla g_{||} = -\epsilon \kappa \mathbf{T} \quad \text{and} \quad \nabla f_{||} = p_2 \mathbf{T}. \quad (3.12)$$

We may then use equations (2.7a,b) in the asymptotic region to conclude that

$$\begin{aligned} f_{\text{out}} &= p_1(x - a + \epsilon y) + p_2(y - \epsilon(x - a)) + \hbar \Theta \\ &= p_1 \xi + p_2 \eta + \hbar \Theta \end{aligned} \quad (3.13a)$$

$$g_{\text{out}} = \kappa a - \epsilon \kappa \eta + \frac{p_2}{p_1} \epsilon \kappa \xi \quad (3.13b)$$

where

$$\begin{aligned} \xi &= x - a + \epsilon y \\ \eta &= y - \epsilon(x - a) \end{aligned} \quad (3.14)$$

and $\Theta = \tan^{-1} \frac{-\kappa}{2p_1 + \epsilon p_2}$ is given by (2.13). The solution for g in the asymptotic region is now a function of η and ξ (or x and y) This is in contrast to the previous example of the square barrier. It is intuitively obvious that the probability density decreases in those regions where the barrier is thicker. The spatial variation of g will lead to interesting phenomena when we come to discuss the scattering of a Gaussian wave-packet off this potential in the next section.

Example 3: $U_3(x) = U_1(x)e^{-\epsilon y}$.

In this example we have a barrier of constant thickness, but varying height. The matching conditions for a step-function give the initial conditions for integrating under

the barrier:

$$\begin{aligned}
\nabla f|_{y=0+} &= (0, p_1) \\
\nabla g|_{y=0+} &= (\sqrt{2mV}e^{-\frac{\epsilon y}{2}}, 0) \\
\psi(0^+, y) &= e^{\frac{i p_1 y}{\hbar}} \left[\frac{2p_1}{p_1 + i\sqrt{2mV}e^{-\frac{\epsilon y}{2}}} \right]
\end{aligned} \tag{3.15}$$

The first step in solving equation (2.7a) is to find the integral curves of ∇g . If we write $\dot{\mathbf{x}} = \nabla g$ (cf Euclidean method) then by examining $\dot{\mathbf{x}} = \nabla U$ we see that

$$\begin{aligned}
\dot{y}^2 &= 2mV(e^{-\epsilon y} - e^{\epsilon y_0}) \\
\dot{x}^2 &= 2mV e^{-\epsilon y_0}.
\end{aligned} \tag{3.16}$$

The equation for the integral curves is therefore

$$\frac{dy}{dx} = -\sqrt{e^{-\epsilon(y-y_0)} - 1}. \tag{3.17}$$

This has solution

$$\begin{aligned}
y &= y_0 + \frac{2}{\epsilon} \log \cos \frac{\epsilon x}{2} \\
&\simeq y_0 - \frac{\epsilon x^2}{4}
\end{aligned} \tag{3.18}$$

this latter approximation being valid when $\epsilon x \ll 1$. Note that the form of the integral curves is invariant along the barrier. The curves all asymptote the line $\epsilon x = \pi$, so we will impose $a < \pi/\epsilon$ to ensure that $(\nabla f)^2$ remains small. Now, for these curves, $\frac{dx}{ds} = e^{-\epsilon(y_0-y)/2} = \cos \frac{\epsilon x}{2}$. Hence

$$\begin{aligned}
g &= \int_{x_0}^x \sqrt{2U} ds = \int_{x_0}^x \sqrt{2mV} e^{-\epsilon y/2} \sec \frac{\epsilon x}{2} dx \\
&= \sqrt{2mV} e^{-\epsilon y_0/2} \frac{2}{\epsilon} \tan \frac{\epsilon x}{2} \\
&= \sqrt{2mV} e^{-\epsilon y/2} \frac{2}{\epsilon} \sin \frac{\epsilon x}{2}.
\end{aligned} \tag{3.19}$$

Having found the zeroth order solution for g , we must now apply (2.7b) to find f , using $f = p_1 y$ initially. From (2.7b) we see that f must be constant along integral curves of g , hence

$$f = p_1 \left(y - \frac{2}{\epsilon} \log \cos \frac{\epsilon x}{2} \right). \tag{3.20}$$

From this we may deduce that $(\nabla f)^2 = p_1^2 \sec^2 \frac{\epsilon x}{2}$ and hence

$$(\nabla g)^2 = 2mV e^{-\epsilon y} + p_1^2 \sec^2 \frac{\epsilon x}{2} - 2mE. \quad (3.21)$$

Now we find ourselves in the situation of having a modified equation for the integral curves of ∇g .

$$\begin{aligned} \frac{dy}{dx} &= - \sqrt{\frac{(e^{-\epsilon(y-y_0)} - 1)}{1 - \frac{E}{V} e^{\epsilon y_0} + \frac{p_1^2}{2mV} e^{\epsilon y_0} \sec^2 \frac{\epsilon x}{2}}} \\ &= - \sqrt{e^{-\epsilon(y-y_0)} - 1} \left[1 + \frac{E}{V} e^{\epsilon y_0} - \frac{p_1^2}{4mV} e^{\epsilon y_0} \sec^2 \frac{\epsilon x}{2} \right]. \end{aligned} \quad (3.22)$$

Setting

$$X = x \left(1 + \frac{E}{V} e^{\epsilon y_0} \right) - \frac{p_1^2}{2\epsilon mV} e^{\epsilon y_0} \tan \frac{\epsilon x}{2}, \quad (3.23)$$

we transform (3.22) back into (3.17), with x replaced by X . Hence

$$y = y_0 + \frac{2}{\epsilon} \log \cos \frac{\epsilon X}{2} \quad (3.24)$$

are the new integral curves, and

$$\begin{aligned} g &= \int_{x_0}^x \sqrt{2mV} e^{-\epsilon y_0/2} \sec \frac{\epsilon X}{2} \sqrt{1 + \frac{p_1^2}{2mV} e^{\epsilon y_0}} ds \\ &= \int_{X_0}^X \sqrt{2mV} e^{-\epsilon y_0/2} \sec^2 \frac{\epsilon X}{2} \left(1 + \frac{p_1^2}{2mV} e^{\epsilon y_0} \right) dX \\ &= \sqrt{2mV} e^{-\epsilon y/2} \sin \frac{\epsilon X}{2} \left(1 + \frac{p_1^2}{2mV} e^{\epsilon y} \sec \frac{\epsilon X}{2} \right) \end{aligned} \quad (3.25)$$

is the new g .

Having now verified the stability of our solution, for calculational brevity we will now retain only the leading order parts of f and g in what follows. We must now match the wave-function across $x = a$. We know that $f, g, \frac{\partial f}{\partial y}, \frac{\partial g}{\partial y}$ all match continuously across the boundary. In particular

$$\begin{aligned} \frac{\partial f}{\partial y} &= p_1 \\ \frac{\partial g}{\partial y} &= -\sqrt{2mV} e^{-\frac{\epsilon y}{2}} \sin \frac{\epsilon a}{2} \end{aligned} \quad (3.26)$$

at $x = a^+$. Using our matching conditions, if we let $p_x = (\frac{\partial f}{\partial x} + i \frac{\partial g}{\partial x})$ then

$$\begin{aligned} p_x^2 &= 2E - (p_1 - i\sqrt{2mV}e^{-\frac{\epsilon y}{2}} \sin \frac{\epsilon a}{2})^2 \\ &= p_1^2 + 2mV e^{-\epsilon y} \sin^2 \frac{\epsilon a}{2} + 2ip_1 \sqrt{2mV} \sin \frac{\epsilon a}{2} e^{-\frac{\epsilon y}{2}} \end{aligned} \quad (3.27)$$

There are two limits in which information can readily be extracted:

$$(a) \sqrt{\frac{E}{U}} \gg \epsilon a$$

In this case the barrier is very slowly varying with respect to the other scales in the problem (although not necessarily with respect to \hbar), and the asymptotic régime is clearly identified as $(\nabla g)^2 \ll (\nabla f)^2$. Clearly we may take $\sin \frac{\epsilon a}{2} \sim \frac{\epsilon a}{2}$, so that to order $\frac{\epsilon a}{\sqrt{E/U}}$ we have

$$p_x = p_1 + i \frac{\epsilon a p_1}{2p_1} \sqrt{2mV} e^{-\frac{\epsilon y}{2}} \quad (3.28)$$

Solving for f and g in the asymptotic region can be achieved by following the same procedure as under the barrier. In this case we first solve for f and then demand that g is constant along the integral curves of ∇f . This gives that

$$f = p_1(x - a) + p_2(y - \frac{2}{\epsilon} \log \cos \frac{\epsilon a}{2}) \quad (3.29a)$$

$$g = \sqrt{2mV} a e^{-\frac{\epsilon}{2}[y - \frac{p_2}{p_1}(x - a)]} \quad (3.29b)$$

These expressions are valid in the region $1 \gg \epsilon[y - \frac{p_2}{p_1}(x - a)] \gg \log \epsilon$.

$$(b) \sqrt{\frac{E}{U}} \ll \sin \frac{\epsilon a}{2}$$

In this case we have

$$p_x \approx \sqrt{2mV} e^{-\frac{\epsilon y}{2}} \sin \frac{\epsilon a}{2} + ip_2 \quad (3.30)$$

In this limit one can ignore the energy term in comparison with $(\nabla f)^2, (\nabla g)^2$ and the WKB equations for f, g become equivalent to the Cauchy-Riemann equations. We can use this to find an approximate solution for f and g in the region $x > a$. If $g = g(a, y)$ and $f = f(a, y)$ on the boundary then letting $z = y + i(x - a)$ we may write

$$\begin{aligned} g &= \text{Reg}(a, z) + \text{Im}f(a, z) = \frac{2}{\epsilon} \sqrt{2mV} \sin \frac{\epsilon a}{2} \cos \frac{\epsilon(x - a)}{2} e^{-\frac{\epsilon y}{2}} + p_2(x - a) \\ f &= -\text{Im}g(a, z) + \text{Re}f(a, z) = \frac{2}{\epsilon} \sqrt{2mV} \sin \frac{\epsilon a}{2} \sin \frac{\epsilon(x - a)}{2} e^{-\frac{\epsilon y}{2}} + p_2(y - \frac{2}{\epsilon} \log \cos \frac{\epsilon a}{2}) \end{aligned} \quad (3.31)$$

At this point let us make a few remarks on the form of this solution. Near the barrier the wave-function dies off doubly exponentially rapidly as $y \rightarrow -\infty$, where the barrier is highest. This is not surprising since the barrier is exponentially rapidly growing here. However what is interesting is that the solution does not seem to make sense for $x \rightarrow a + \pi/\epsilon$ as $g \rightarrow 0$ here, making the wave-function (doubly) exponentially enhanced relative to its value near the barrier. This can be understood by looking at the integral curves of ∇f , which asymptote $x = a + \pi/\epsilon$. As we approach this line, we cross integral curves of ∇f which emanated from $x = a$ at larger and larger values of y , in particular where $\sqrt{E/U} \sim \epsilon a$, where approximation (b) is no longer valid. Thus the solution (3.31) cannot be extrapolated to $x \sim a + \pi/\epsilon$, and can only be regarded as a solution close to the barrier. However, it is interesting in that it deals with a régime in which the barrier is rapidly varying in height.

4. Scattering of Gaussian wave-packets

We are interested in understanding what happens when a classical particle scatters off the sort of potentials we have been considering. So far, we have given a solution for incoming plane waves scattering off such potentials. The linearity of Schrödinger's equation enables us to add these solutions together in order to find time-dependent solutions. We will be interested in considering solutions for which the incoming wave is a Gaussian wave-packet, since this can be thought of as representing a classical particle. After some introductory remarks we shall examine the solution for a Gaussian wave-packet scattering off each of the potentials considered in the last section.

Briefly, we review Gaussian wave-packets to establish notation. Let us consider a solution to the one-dimensional Schrödinger equation, which at time $t = 0$ has the form

$$\Psi(x, 0) = \lambda^{\frac{1}{4}} \pi^{-\frac{1}{4}} e^{\frac{ip_1 x}{\hbar}} e^{-\frac{\lambda x^2}{2}} \quad (4.1)$$

To find $\Psi(x, t)$ we first take the Fourier transform

$$\begin{aligned} F(k) &= \frac{1}{2\pi} \int dx \lambda^{\frac{1}{4}} \pi^{-\frac{1}{4}} e^{i(\frac{p_1}{\hbar} - k)x} e^{-\frac{\lambda x^2}{2}} \\ &= 2^{-\frac{1}{2}} \pi^{-\frac{3}{4}} \lambda^{-\frac{1}{4}} \exp \left\{ -\frac{(\frac{p_1}{\hbar} - k)^2}{2\lambda} \right\} \end{aligned} \quad (4.2)$$

Then we have that

$$\begin{aligned} \Psi(x, t) &= \int d\left(\frac{k}{\hbar}\right) F\left(\frac{k}{\hbar}\right) e^{\frac{ikx}{\hbar}} e^{-\frac{i\hbar^2 k^2 t}{2m}} \\ &= (2A)^{-\frac{1}{2}} \hbar^{-1} \pi^{-\frac{1}{4}} \lambda^{-\frac{1}{4}} \exp \left\{ -\frac{(x - \frac{p_1 t}{m})^2}{4\hbar^2 A} - \frac{ip_1^2 t}{2m\hbar} + \frac{ixp_1}{\hbar} \right\} \end{aligned} \quad (4.3)$$

where $A = \frac{1}{2\lambda\hbar^2} + \frac{it}{2m\hbar}$. This solution represents a Gaussian wave-packet with momentum p_1 . The wave-packet has $\langle \Delta x^2 \rangle = 2\hbar^4\lambda|A|^2$ and $\langle \Delta k^2 \rangle = \frac{1}{2}\lambda\hbar^2$. The modulus of A is smallest at $t = 0$ and at this time the wave-packet is minimal. The wave-packet begins to spread appreciably for $|t| > \frac{m}{\lambda\hbar}$.

People are generally interested in two types of wave packet: those extremely peaked in momentum space (λ of order unity) and those equally spread in position and momentum space ($\lambda = O(\hbar^{-1})$). Notice that even in this latter category, the wave packets are still very sharply ($\sim \hbar$) peaked in momentum space. In the first case, the packet, although comparatively diffuse in x -space, maintains its shape for $t < \hbar^{-1}$, whereas in the second case, the packet starts to spread for t of order unity (although the spread is still of order \hbar); this is quite sufficient. We will therefore assume that $\lambda\hbar$ is at most of order unity.

In the previous section we obtained the solution for a plane wave scattering off three different potentials, what is now required is that we take the appropriate linear combinations of these solutions so that the composite describes an incident wave-packet which can be interpreted as a classical particle. This is simply a product of the solutions described above; that is

$$\Psi_{\text{in}}(x, y, t) = \frac{1}{2\hbar^2 A \sqrt{\pi\lambda}} e^{-\frac{iEt}{\hbar}} \exp \left\{ -\frac{1}{4\hbar^2 A} \left[\left(x - \frac{p_1 t}{m}\right)^2 + \left(y - \frac{p_2 t}{m}\right)^2 \right] + \frac{ixp_1}{\hbar} + \frac{iyp_2}{\hbar} \right\} \quad (4.4)$$

where $E = \frac{1}{2m}(p_1^2 + p_2^2)$. This describes a wave packet with momentum (p_1, p_2) hitting the origin at $t = 0$. The momentum profile of the wave-function has the form

$$F\left(\frac{k_1}{\hbar}, \frac{k_2}{\hbar}\right) = \frac{1}{2\pi\hbar^2 \sqrt{\pi\lambda}} e^{-\frac{1}{2\lambda\hbar^2}[(k_1 - p_1)^2 + (k_2 - p_2)^2]} \quad (4.5)$$

In order to find the emergent wave-function we integrate

$$\Psi_E(x, y, t) = \iint dk_1 dk_2 F\left(\frac{k_1}{\hbar}, \frac{k_2}{\hbar}\right) \psi_{\text{out}}(k_i, x, y) e^{\frac{-i(k_1^2 + k_2^2)t}{2m\hbar}} \quad (4.6)$$

where

$$\psi_{\text{out}} \propto e^{i(f_{\text{out}} + ig_{\text{out}})} \quad (4.7)$$

is the approximate form of the outgoing wave function calculated in section three. We may write this integral in the form

$$\Psi_E(x, y, t) = \frac{1}{2\pi\hbar^2 \sqrt{\pi\lambda}} \iint dk_1 dk_2 e^{\Lambda/\hbar} \quad (4.8)$$

where

$$\Lambda(x, y, k_1, k_2, t) = if_{\text{out}} - g_{\text{out}} - \frac{1}{2\lambda\hbar}(k_i - p_i)^2 - \frac{it}{2m}k_i^2. \quad (4.9)$$

We use a saddle point method to calculate this integral making the exponent stationary with respect to k_1, k_2 . We are interested in the trajectory of the peak of the wave packet, the position of which is given by $\nabla \text{Re}\Lambda = 0$. We then use the set of equations

$$\frac{\partial \Lambda}{\partial k_i} = 0 \quad (4.10a)$$

$$\nabla \text{Re}\Lambda = 0 \quad (4.10b)$$

to determine the trajectory of the outgoing wave packet.

Having now outlined the general procedure, let us return to our three examples, investigating the behaviour of a Gaussian wave packet as it hits each in turn.

Example 1: $U(x) = V\Theta(x)\Theta(a-x)$.

Here we substitute in (4.6) the outgoing wave function from equation (3.2):

$$\psi_{\text{out}} = T(k_1)e^{ik_1 x/\hbar} \quad (4.11)$$

where T is the transmission coefficient in eq(3.3b). Integrating over k_2 merely inverts the Fourier transform in the y -direction since T is independent of y and the integral over the x -momentum is peaked about some k_x close to $p_1 \ll U$. We therefore approximate T by

$$T(k_1) \sim \frac{2k_x \kappa(k_x)}{mV} \exp \left\{ -\frac{ik_1 a}{\hbar} - \frac{\kappa(k_1)}{\hbar} - \frac{i\Theta(k_1)}{\hbar} \right\}. \quad (4.12)$$

This now simplifies the expression (4.9) for the exponent:

$$\Lambda(x, t, k_1) = ik_1(x - a) - \frac{1}{2\lambda\hbar}(k_1 - p_1)^2 - \frac{it}{2m}k_1^2 - \kappa a - i\Theta(k_1). \quad (4.13)$$

Using the saddle-point approximation we expect that

$$\Psi_E(x, y, t) \propto \exp \left\{ -\frac{1}{4\hbar^2 A} \left(y - \frac{p_2 t}{m} \right)^2 + \frac{ip_2 y}{\hbar} - \frac{ip_2^2 t}{2m\hbar} \right\} e^{\frac{\Lambda(x, t, k_x)}{\hbar}} \quad (4.14)$$

where

$$0 = \frac{\partial \Lambda}{\partial k_1} \Big|_{k_x} = i(x - a) - \frac{1}{\lambda\hbar}(k_x - p_1) - \frac{ik_x t}{m} + \frac{ak_x}{\sqrt{2mV - k_x^2}} - i\Theta'(k_x) \quad (4.15)$$

In order to find the trajectory of the peak of the emergent wave packet, we combine this information with (4.10b) (which simply reduces to $\text{Im}k'_x = 0$). Doing this, we find that along the peak

$$x = a + \Theta' + \frac{k'_x t}{m} \quad (4.16)$$

where k'_x , the momentum of the peak, is determined by the real part of (4.11), which we may expand to order $\sqrt{E/V}$ to obtain

$$k'_x = p_1 \left(1 + \frac{a\lambda\hbar}{\sqrt{2mV}} \right) \quad (4.17)$$

This, together with the equation giving the peak in the y -direction which is obviously $y = \frac{p_2 t}{m}$ suggests that the peak emerges at time $t_e = -\Theta' m / k'_x = O(\hbar)$ at $(a, \frac{2p_2\hbar}{k'_x \kappa})$, and travels subsequently in a straight line.

We have been deliberately obscure about the actual value of Θ' (and hence t_e) since it would be misleading to advertise this as the *actual* tunnelling time when there is considerable debate on this topic¹¹, indeed, as we shall see in the next two examples, taking this quantity seriously as a tunnelling time would lead to some interesting physical dilemmas. This time is called the *phase time*^{15,16} of the tunnelling process, and is really only well defined asymptotically, well after the scattering/tunnelling process has been completed. One way of seeing why this must be so is to recall that the distortions of the wave packet close to the barrier make 'definitions' such as 'when the particle hits the barrier' subjective at best, meaningless at worst. Our reason for including this term is twofold. First we wish to emphasise the physical, quantum mechanical nature of tunnelling. Secondly, in the next two examples, we find factors in t_e due to the variation of the potential and we would like to compare the two factors.

Example 2: $U_2(x) = V\Theta(x)\Theta(a - x + \epsilon y)$.

Having worked through the first example in some detail, we now summarise the steps for this example. Using (3.13), we may write the exponent (4.9) as

$$\Lambda(\xi, \eta, k_1, k_2, t) = -\frac{(k_i - p_i)^2}{2\lambda\hbar} - \frac{itk_i^2}{2m} - \kappa a + \epsilon\kappa\eta - \frac{k_2}{k_1}\epsilon\kappa\xi + i(k_1\xi + k_2\eta + \Theta\hbar). \quad (4.18)$$

where ξ and η are given by (3.15). Making this stationary with respect to the k_i yields the two (complex) equations:

$$\begin{aligned} -\frac{1}{\lambda\hbar}(k_x - p_1) - \frac{it}{m}k_x + \frac{k_x a}{\kappa} - \epsilon\left(\frac{k_x \eta}{\kappa} - \frac{k_y \kappa \xi}{k_x^2} - \frac{k_y \xi}{\kappa}\right) + i(\xi + \Theta_{,1}\hbar) &= 0 \\ -\frac{1}{\lambda\hbar}(k_y - p_2) - \frac{it}{m}k_y - \frac{\epsilon\kappa\xi}{k_x} + i(\eta + \Theta_{,2}\hbar) &= 0 \end{aligned} \quad (4.19)$$

For the trajectory of the wave packet we use (4.10b) and (4.18) to find

$$\text{Im}k'_x = -\epsilon \text{Re} \frac{k'_y \kappa}{k'_x} \quad (4.20a)$$

$$\text{Im}k'_y = \epsilon \text{Re} \kappa. \quad (4.20b)$$

Now we have a situation in which the momentum dominating the integral is complex. Writing k'_x for $\text{Re}k'_x$, and substituting from (4.20) for $\text{Im}k'_x$, and similarly for k'_y , the equations for the emergent wave peak can be seen to be

$$\xi = -\Theta_{,1} \hbar + \frac{k'_x t}{m} - \frac{k'_y}{k'_x} \hat{\epsilon} + \frac{k'_y}{k'_x} \epsilon a \quad (4.21a)$$

$$\eta = -\Theta_{,2} \hbar + \frac{k'_y t}{m} + \hat{\epsilon} \quad (4.21b)$$

where

$$\hat{\epsilon} = \frac{\epsilon \kappa}{\lambda \hbar} \quad (4.22a)$$

$$k'_x = p_1 \left(1 + \frac{a \lambda \hbar}{\kappa} \right) \quad (4.22b)$$

$$k'_y = p_2 \quad (4.22c)$$

Thus we see that the packet emerges from under the barrier at a time and displacement given by

$$t_e = \frac{m}{k'_x} \left[\Theta_{,1} \hbar + \hat{\epsilon} \frac{k'_y}{k'_x} (1 - a \lambda \hbar / \kappa) \right] \quad (4.23a)$$

$$\eta_e = \hbar \left(\frac{k'_y}{k'_x} \Theta_{,1} - \Theta_{,2} \right) + \hat{\epsilon} \left(1 + \frac{k'^2_y}{k'^2_x} (1 - a \lambda \hbar / \kappa) \right) \quad (4.23b)$$

subsequently travelling along the straight line

$$\eta = \frac{k'_x \xi}{k'_y} + \hat{\epsilon} \left(1 + \frac{k'^2_y}{k'^2_x} (1 - a \lambda \hbar / \kappa) + O(\hbar) \right) \quad (4.23c)$$

with a damping relative to the incident Gaussian of

$$e^{-\kappa(a - \epsilon \eta_e)/\hbar} \simeq e^{-\kappa x_{out}/\hbar}. \quad (4.23d)$$

There are several interesting differences with the previous example. The first is that the tunnelling time can now be negative! This peculiarity arises for a simple physical reason, the fact that the most energetically favourable time for the Gaussian to tunnel is not necessarily when the peak hits the barrier. Tunnelling amplitudes depend exponentially on the size of the barrier, therefore it is more favourable to tunnel when the barrier is thinner or lower. On the other hand, the probability density along $x = 0$ is damped by an exponential factor depending upon how far away that point is from the peak of the Gaussian. Clearly there will be a pay off between these two factors which *may* mean that it is more energetically favourable for the fringe of the Gaussian to tunnel, rather than its peak.

The second thing to notice is that the wave packet emerges on the other side of the barrier at $\eta = \eta_e$, somewhat 'downstream' of where one might expect it. The two possibilities for emergence would be the perpendiculars from either the start of the barrier, or its end, that is, $\eta = 0$ or $\eta = a\epsilon$. Neither of these naive choices are equal to η_e . This shift has the same physical origin as the unusual t_e .

Finally, we should remark that the incoming and outgoing momentum are not quite parallel, since the (x, y) and (ξ, η) coordinate systems do not quite coincide.

Example 3: $U_3(x) = U_1(x)e^{-\epsilon y}$.

We shall now discuss the problem of scattering a Gaussian wave-packet off a barrier of variable height. This problem is much closer to the sort found in inflationary models. As before, the emergent wave-function will be the superposition

$$\psi_E(x, y, t) = \iint dk_1 dk_2 F\left(\frac{k_1}{\hbar}, \frac{k_2}{\hbar}\right) \psi_{\text{out}}(k_i, x, y) e^{-\frac{i\hbar_2 y_0}{\hbar} - \frac{iEt}{\hbar}} \quad (4.24)$$

where we include the factor of $e^{-\frac{i\hbar_2 y_0}{\hbar}}$ so that the wave packet hits the barrier at $(0, y_0)$ rather than the origin. Recall ψ_{out} was calculated in two separate limits. We now calculate the outgoing peak trajectory in each case.

$$(a) \sqrt{\frac{E}{U}} \gg \epsilon a$$

In this case, from (3.29), we find that Λ is equal to

$$\Lambda = -\frac{(k_i - p_i)^2}{2\lambda\hbar} - \frac{itk_i^2}{2m} + i(k_1(x-a) + k_2(y-y_0 - \frac{2}{\epsilon} \log \cos \frac{\epsilon a}{2})) - \sqrt{2mV} a e^{-\frac{\epsilon}{2}(y-y_0 - \frac{\hbar^2}{k_1^2}(x-a))} \quad (4.25)$$

Making this stationary with respect to the k_i gives

$$\begin{aligned} -\frac{1}{\lambda\hbar}(k_x - p_1) - \frac{it}{m}k_x + i(x - a) + \frac{\epsilon a}{2}\sqrt{2mV}\frac{k_y}{k_x^2}(x - a) &= 0 \\ -\frac{1}{\lambda\hbar}(k_y - p_2) - \frac{it}{m}k_y + i\left(y - \frac{2}{\epsilon}\log\cos\frac{\epsilon a}{2}\right) + \frac{\epsilon a}{2}\sqrt{2mV}\left(1 - \frac{x - a}{k_x}\right) &= 0 \end{aligned} \quad (4.26)$$

As before, we use (4.10b) to find the trajectory of the peak of the wave packet

$$\text{Im}k'_x = -\frac{\epsilon a}{2}\sqrt{2mV}\text{Re}\frac{k'_y}{k'_x} \quad (4.27a)$$

$$\text{Im}k'_y = \frac{\epsilon a}{2}\sqrt{2mV} \quad (4.27b)$$

Again, the momentum dominating the integral is complex. Writing k'_x for $\text{Re}k'_x$ etc. as before, the equations for the emergent wave peak can be seen to be

$$(x - a) = \frac{k'_x t}{m} + \frac{k'_y}{k'_x}\hat{\epsilon} \quad (4.28a)$$

$$y = y_0 + \frac{2}{\epsilon}\log\cos\frac{\epsilon a}{2} + \frac{k'_y t}{m} + \hat{\epsilon} \quad (4.28b)$$

where

$$\hat{\epsilon} = \frac{\epsilon a\sqrt{2mV}}{2\lambda\hbar} \quad (4.29a)$$

$$k'_x = p_1 \quad (4.29b)$$

$$k'_y = p_2 + \frac{\epsilon a\lambda\hbar}{2}\sqrt{2mV} \quad (4.29c)$$

Therefore the packet emerges from under the barrier at

$$t_e = \frac{m\hat{\epsilon}k'_y}{k_x'^2} \quad (4.30a)$$

$$y_e = y_0 + \frac{2}{\epsilon}\log\cos\frac{\epsilon a}{2} + \hat{\epsilon}\left(1 + \frac{k_y'^2}{k_x'^2}\right) \quad (4.30b)$$

subsequently travelling along the straight line

$$y = y_0 + \frac{2}{\epsilon}\log\cos\frac{\epsilon a}{2} + \frac{k'_x}{k'_y}(x - a) + \hat{\epsilon}\left(1 + \frac{k_y'^2}{k_x'^2}\right) \quad (4.30c)$$

with a damping relative to the incident Gaussian of

$$e^{-\sqrt{2mV}ae^{-\frac{1}{2}v_0/\hbar}} \quad (4.30d)$$

Thus, as in the previous example, the tunnelling time once more can be negative (for the same reason) and the peak of the transmitted wave packet emerges somewhat downstream from where we might have expected.

$$(a) \sqrt{\frac{E}{U}} \ll \epsilon a$$

In this case, from (3.31), we obtain

$$\Lambda = -\frac{2}{\epsilon} \sqrt{2mV} \sin \frac{\epsilon a}{2} e^{i \frac{\epsilon(y+(a-a))}{2}} + ik_2(y - y_0 - \frac{2}{\epsilon} \log \cos \frac{\epsilon a}{2} + i(x - a)) - \frac{(k_i - p_i)^2}{2\lambda\hbar} - \frac{ik_i^2 t}{2m} \quad (4.31)$$

Using saddle-point methods to evaluate this integral we arrive at the solution

$$\begin{aligned} y &= y_0 + \frac{2}{\epsilon} \log \cos \frac{\epsilon a}{2} + e^{-\frac{1}{2}v_0/\hbar} \sqrt{2mV} \sin \frac{\epsilon a}{2} \left(\frac{1}{\lambda\hbar} \cos \frac{\epsilon(x-a)}{2} + \frac{t}{m} \sin \frac{\epsilon(x-a)}{2} \right) \\ x &= a + \frac{p_2}{\lambda\hbar} + e^{-\frac{1}{2}v_0/\hbar} \sqrt{2mV} \sin \frac{\epsilon a}{2} \left(-\frac{1}{\lambda\hbar} \sin \frac{\epsilon(x-a)}{2} + \frac{t}{m} \cos \frac{\epsilon(x-a)}{2} \right) \end{aligned} \quad (4.32)$$

so that the peak emerges at $x = a$ at a time and position given by

$$t_e = -\frac{p_2 e^{\epsilon v/2}}{\lambda\hbar \sqrt{2mV} \sin \frac{\epsilon a}{2}} \quad (4.33a)$$

$$y_e = y_0 + \frac{2}{\epsilon} \log \cos \frac{\epsilon a}{2} + \frac{e^{-\frac{1}{2}v_0/\hbar} \sqrt{2mV}}{\lambda\hbar} \sin \frac{\epsilon a}{2} \quad (4.33b)$$

As in the previous examples there are three terms which contribute to the value of y at which the particle emerges: its initial position, the shift to this due to the curvature of the ∇g integral curves under the barrier and a term which depends on the spread λ . Again, the time at which the peak emerges can be positive or negative depending on the sign of p_2 .

5. Conclusions.

In this paper we have generalised existing methods for calculating tunnelling processes to allow for complex momentum. This allows us to calculate tunnelling amplitudes in a wider class of potentials. We started by reviewing the BBW approach, then described how to generalise this to include complex momentum. The problem of solving under the

barrier was made tractable by assuming that the energy of the wave function was small compared with the height of the barrier. The matching conditions we derived by imposing continuity of the wave function allowed us to transport real momentum under the barrier and imaginary momentum beyond.

In section 3 we applied this method to three examples: a square barrier for which we knew the exact solution, a step function of varying width, and then one of varying height. We found that the outgoing momentum was not necessarily parallel to the incoming momentum, a feature that we expect for generic barriers. Examining the scattering of Gaussians against these barriers allowed us to follow a wave packet tunnelling; probably a more realistic physical scenario. In recapping the square barrier case, we could illustrate the origin of one definition of tunnelling time, the phase time. We used this to explore the effect of barrier variation. This, as it turned out, was quite significant. Both in the case of the step barrier with varying height and that of varying width we found large corrections to t_e and a shift in the place of emergence of the wave packet into the asymptotic régime. These turned out to have a simple physical origin. It is incorrect to assume that it is the peak of the incoming packet that dominates the emergent wave-function, and that tunnelling takes place when this peak is next to the barrier. Tunnelling is an exponentially suppressed phenomenon, and therefore it is far more favourable to tunnel where the barrier is smaller, even if the impinging probability density there is not a maximum.

The last two examples we considered suggest that the definition of 'phase time' as it stands is not a good definition of tunnelling time since it assumes that the tunnelling process starts when the peak hits the barrier. It is possible that some modification of this description would give sensible results, compatible with the uncertainty principle for energy and time, although such a modification would naturally weaken the status of phase time. Unfortunately, we are not able to shed any light on whether some alternative definitions of tunnelling times¹⁷⁻¹⁹ are any better.

We restricted ourselves to the examples discussed since they illustrate the salient features of multi-dimensional tunnelling without too great calculational complexity. However, it was the cosmological applications of complex momentum tunnelling that originally interested us, and these involve tunnelling processes from semi-localised states in field theory. The problem of calculating a tunnelling rate from a state localised in the x -direction should represent one step up in complexity from our examples and is currently being calculated. The problem of applying these ideas to field theory would involve translating the techniques presented here into the functional Schrödinger picture. This may prove to be very problematic, although clearly that is the next step in solving the two field problem.

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